Hexachloropropene

1888-71-7 | DTXSID7062039

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -34.7 °C

Global applicability domain: Inside

Local applicability domain index: 6.21e-01

Confidence level: 3.08e-01

Nearest Neighbors from the Training Set

Image not found
Hexachloropropene
Measured: -72.9
Predicted: -34.7

Image not found
Hexachloro-1,3-butadiene
Measured: -21.0
Predicted: -20.7

Image not found
Hexachloroethane
Measured: 187
Predicted: 118

Image not found
Tetrachloroethylene
Measured: -22.3
Predicted: -13.3

Image not found
Hexachlorocyclopentadiene
Measured: -9.00
Predicted: 2.05